Tetrachloroethylene

127-18-4 | DTXSID2021319

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 21.2 days

Global applicability domain: Outside

Local applicability domain index: 4.93e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found

Cyclohexane

Measured: 50.0 Predicted: 34.7

Image not found
Cyclopentane

Measured: 50.0

Predicted: 35.5

Image not found

Benzene

Measured: 6.00 Predicted: 10.3

Image not found

2,2,3-Trimethylbutane

Measured: 6.00 Predicted: 10.7

Image not found

2,3,4-Trimethylpentane

Measured: 15.0 Predicted: 13.9